Carcinogenic Potency Database (CPDB)

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Function

The file "CPDBChemical_Summary.xls" and folders described herein contain essential data used to support the Carcinogenic Potency Database (CPDB) formerly published at https://toxnet.nlm.nih.gov/cpdb/. The CPDB was a unique and widely used international resource of qualitative and quantitative data from 6540 chronic, long-term animal cancer tests on 1547 chemicals. It included data from studies in rats, mice, hamsters, dogs, and nonhuman primates, and provided easy access to positive as well as negative bioassay results that had been published in the general literature or by the National Cancer Institute/National Toxicology Program over a span of 50 years, through 2004 The CPDB helped standardize the diverse literature of cancer bioassays that vary widely in protocol, histopathological examination and nomenclature, and in methods for reporting data depending on the author's choices of information to be included.

Files/Folders

- a) CPDBChemical_Summary.xls: An Excel formatted summary of the carcinogenicity results of all 1547 chemicals in CPDB. The file contains a tab for each species group.
- b) <u>Individual Chemical Pages</u>: This folder contains all 1547 chemicals used in the CPDB in PDF format. The pages are divided into Cancer Test Summary, Experiments and Citations in CPDB, and plots/tables of the data. All *primary* linked data within the chemical pdfs are contained in the <u>Supporting Documents</u> folder unless otherwise specified. The links within the pdfs are not functional, however the names of the specific pdf for each link are as follows:
 - Carcinogenic Potency Database: "index-2.pdf"
 - TD₅₀: "td50.pdf"
 - Harmonic Mean: "td50harmonicmean.pdf"
 - Criteria for inclusion of experiments: "methods.pdf"
 - Standardization of average daily dose levels: "methods.pdf"
 - TD50 estimation for a standard lifespan: "methods.pdf"
 - Methods: "methods.pdf"
 - Strain: "strain.pdf"
 - Site: "tissue.pdf"
 - Path: "tumor.pdf"
 - Guide: "condensedplot.pdf"
 - Help: "Zoom.pdf"
 - Species: "species.pdf"
 - Sex: "sex.pdf"
 - Route: "route.pdf"
 - Xpo+Xpt: "xpoxpr.pdf"
 - PaperNum: "papernum.pdf"
 - Literature Reference: "biblio.pdf"
 - Notes: "note.pdf"
 - DR: "curve.pdf"
 - Pval: "confidence.pdf"
 - AuOp: "opinion.pdf"
 - LoConf: "confidence.pdf"
 - UpConf: "confidence.pdf"
 - Brkly Code: "Berkeley.pdf"
 - USEPA Distributed Structure-Searchable Toxicity (DSSTox) Database: new link https://www.epa.gov/chemical-research/distributed-structure-searchable-toxicity-dsstox-database
 - National Library of Medicine ChemIDPlus: active link http://chem.sis.nlm.nih.gov/chemidplus/
 - Summary Table: "chemicalsummary.pdf"

- Full CPDB: "condensedplot.pdf"
- Summary Table by Target Organ: "pathology.table.pdf"
- several formats: "index-2.pdf"
- A plot: "database.pdf"
- A Screen version: "condensedplot.pdf"
- Excel version: "CPDB-tab.pdf"
- Tab-separated versions: "CPDB-tab.pdf"
- Supplementary Dataset: "CPDBsupplementary-tab.pdf"
- Excel spreadsheet: "ltd10chemicalsummary.pdf"
- year: "listofpubs.year.pdf"
- topic: "listofpubs.topic.pdf"
- c) <u>Resources</u>: This folder contains datasets, data plots, appendices, summaries and supporting documents organized by subfolders.
 - <u>Individual_Chemical_Pages</u>: A copy of the aforementioned folder.
 - <u>Plot</u>: This folder contains the two files of the left and right sides of the plotted data in PDF format in addition to 12 appendices and two bibliography files in PDF format
 - Plotted data
 - o plot-left.pdf: Left side of the plot
 - o plot-right.pdf: Right side of the plot
 - Appendices
 - o species.pdf: Codes for animal species
 - strain.pdf: Codes for animal strain
 - o route.pdf: Codes for route of administration
 - site.pdf: Codes for anatomical locations
 - o tumor.pdf: Codes for histopathology
 - note.pdf: Codes for notes
 - o curve.pdf: Codes for dose-response curve and plot symbols
 - o statmethods.pdf: Statistical methods for estimating TD₅₀
 - berkeley.pdf: Codes for Berkeley NCI/NTP Bioassays
 - o journal.pdf: Codes for journal articles
 - o synonyms.pdf: Synonyms for chemicals in CPDB
 - Bibliographies
 - NClbiblio.pdf: Bibliography of technical reports of the National Cancer Institute/ National Toxicology Program
 - biblio.pdf: General literature

- <u>Screen_Version</u>: This folder a condensed version of the plotted data viewable in a single in PDF format in addition to 12 appendices and 2 bibliography files in PDF format.
 - Plotted data
 - CPDBcondensed.pdf: Entire plot of CPDB chemicals
 - Appendices
 - o species.pdf: Codes for animal species
 - o strain.pdf: Codes for animal strain
 - o route.pdf: Codes for route of administration
 - site.pdf: Codes for anatomical locations
 - tumor.pdf: Codes for histopathology
 - note.pdf: Codes for notes
 - o curve.pdf: Codes for dose-response curve and plot symbols
 - o statmethods.pdf: Statistical methods for estimating TD₅₀
 - o berkeley.pdf: Codes for Berkeley NCI/NTP Bioassays
 - o journal.pdf: Codes for journal articles
 - o synonyms.pdf: Synonyms for chemicals in CPDB
 - Bibliographies
 - NClbiblio.pdf: Bibliography of technical reports of the National Cancer Institute/ National Toxicology Program
 - biblio.pdf: General literature
- <u>Tab-seperated Version</u>: This folder contains six main datasets of the CPDB data and six appendices in tab-separated format in addition to the file
 "Documentation for tab.pdf" that delineates the columns in each dataset.
 - Datasets
 - o cpdb.ncintp.tab: All data for NCI/NTP except doses and incidence
 - cpdb.ncintpdose.tab: Dose and incidence data for NCI/NTP
 - o cpdb.lit.tab: All data for literature except: doses and incidence
 - o cpdb.litdose.tab: Dose and incidence data for literature
 - cpdb.chemname.tab: Chemical names, three-letter identification codes and CAS numbers
 - o cpdb.cit.tab: Brief citation to published paper in literature
 - Appendices
 - o cpdb.species.tab: Species code definitions
 - o cpdb.route.tab: Route code definitions
 - o cpdb.strain.tab: Strain code definitions
 - o cpdb.tissue.tab: Tissue code definitions
 - o cpdb.tumor.tab: Tumor histopathology code definitions
 - o cpdb.journal.tab: Journal code definitions

 <u>Excel Version</u>: This folder 6 main datasets of the CPDB data and 6 appendices in Excel format in addition to the file "<u>Documentation_for_Excel.pdf</u>" that delineates the columns in each dataset.

Datasets

- o cpdb.ncintp.tab: All data for NCI/NTP except doses and incidence
- o cpdb.ncintpdose.tab: Dose and incidence data for NCI/NTP
- o cpdb.lit.tab: All data for literature except: doses and incidence
- o cpdb.litdose.tab: Dose and incidence data for literature
- cpdb.chemname.tab: Chemical names, three-letter identification codes and CAS numbers
- o cpdb.cit.tab: Brief citation to published paper in literature

Appendices

- cpdb.species.tab: Species code definitions
- o cpdb.route.tab: Route code definitions
- o cpdb.strain.tab: Strain code definitions
- o cpdb.tissue.tab: Tissue code definitions
- o cpdb.tumor.tab: Tumor histopathology code definitions
- o cpdb.journal.tab: Journal code definitions
- <u>Supplementary Datasets</u>: This folder contains two supplementary datasets available in both tab-separated and Excel formats in addition to the file "CPDB_Supplementary.pdf" that delineates the columns in each dataset. Also included is the file "CPDBsupplementary-tab.pdf" that gives an overview of the supplementary datasets.
 - cpdb.supp.xls: Each row represents a single dose-group (including control) for each experiment in Excel format.
 - cpdb.suppvary.xls: A small dataset that only contains variable dosing. Each row is a dosing protocol within a dose-group in Excel format.
 - cpdb.supp.tab: Each row represents a single dose-group (including control) for each experiment in tab-separated format.
 - cpdb.suppvary.tab: A small dataset that only contains variable dosing.
 Each row is a dosing protocol within a dose-group in tab-separated format.
- <u>Supporting Documents</u>: This folder includes PDF files with information on corresponding links from files in the <u>Individual Chemical Pages</u> folder.
- <u>Summary Table By Chemical</u>: This folder contains a summary of the carcinogenicity results for all 1547 chemicals in the CPDB in three different

formats, listed below. Structures of all chemicals are included in PDF format along with molecular weights, SMILES and InChI codes in both Excel and tabseparated formats.

- Summary Tables
 - CPDBChemical_Summary.xls: An excel formatted summary of the carcinogenicity results of all 1547 chemicals in CPDB. The file contains a tab for each species group.
 - ChemicalTable.pdf: PDF format
 - ChemicalTable.rtf: Rich text format that is easily loadable into a database
- Chemical structures
 - o structure.pdf: Chemical structures of all 1547 chemicals
- Molecular weights, SMILES and InChI codes
 - chemical-structures.xls: Excel format
 - o chemical-structures.tab: Tab-separated format
- <u>Summary Table By Organ</u>: This folder contains results on chemicals in the CPDB that induce tumors in each of 35 target organs in rats, mice, hamsters, monkeys, or dogs in a single PDF file "CPDBPathology.pdf". Also included is the PDF file "pathology.table.pdf" that gives details regarding the summary table.
- <u>Copied website</u>: This folder contains all data from the previously published
 CPDB website except the individual chemical data already included in <u>Individual</u>
 <u>Chemical Pages</u> folder. Note: All original html files have been replaced with pdf files to preserve images that were provided by external links.

Additional Instructions/Information

• Please contact CEBS-Support@mail.nih.gov for additional assistance.